

DESIGN OF GATES FOR QUANTUM COMPUTATION: THE NOT GATE

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Received 17 April 1997

We offer an alternative to the conventional network formulation of quantum computing. We advance the *analog* approach to quantum logic gate/circuit construction. As an illustration, we consider the *spatially extended* NOT gate as the first step in the development of this approach. We derive an explicit form of the interaction Hamiltonian corresponding to this gate and analyze its properties. We also discuss general extensions to the case of certain time-dependent interactions which may be useful for practical realization of quantum logic gates.

1. Introduction

The fundamental physics of reversible quantum-mechanical computation has received much attention recently.¹ Quantum computer is a hypothetical quantum-coherent system that functions as a programmable calculational apparatus. Such a computer will have to be drastically different from its classical counterparts. It will enable solution of certain problems¹ much faster than the classical computer: the quantum interference property yields¹ the fast-factoring (Shor's), as well as certain other fast algorithms. Recent theoretical results have included identification of universal reversible two-bit gates² and advances³ in error correction. There have also been experiments⁴ realizing a simple gate.

Nevertheless, the idea of construction of a macroscopic computer out of a large number of quantum bits (qubits) is elusive⁵ at the present stage of technology. The main obstacle is the sensitivity of coherent quantum evolution and interference to undesirable external interactions such as noise or other failures in operation.^{1,5,6} Even though a number of error correction schemes have been proposed,³ not all types of error can be corrected. This particularly applies to the *analog* nature of quantum computers⁶ which will be addressed below.

Quantum computers are naturally analog in their operation because in order to use the power of quantum interference, one has to allow any linear combination of

the basis qubit states. By analog errors we mean those minor variations in the input and output variables and in the system's dynamics which cannot on their own be identified as erroneous in an analog device because its operation involves continuous values of variables (so that the fluctuated values are as legal as the original ones). By noise errors we mean those that result from single-event problems with device operation, or from external influences, or from other failures in operation. In the quantum case the latter errors also include the decoherence effects due to influences of the environment.

Error-correction techniques can handle the noise errors but not the analog errors. Indeed consider a state $\alpha|1\rangle + \beta|0\rangle$ and a nearby state $\alpha'|1\rangle + \beta'|0\rangle$, where α' is close to α , while β' is close to β . Here $|1\rangle$ and $|0\rangle$ denote the basis qubit or spin states in the notation reminiscent of the classical bit states 1 and 0. Both linear-superposition states are equally legal as input or output quantum states. Furthermore in the conventional picture of a quantum computer¹ which assumes a network of a multitude of simple gate-units each being controlled externally, the analog errors can proliferate and be magnified in each step of the computation.

In this work we therefore adopt a view typical of the “classical” analog computer approach, of designing the computer as a *single unit* performing in one-shot a complex logical task instead of a network of simple gates each performing a simple “universal-set” logical function. In this case the computer as a whole will still be subject to analog errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled. Indeed, quantum (and more generally reversible) computation must be externally timed: the time scale of the operation of each gate is determined by the interactions rather than by the relaxation processes as in the ordinary computer. Furthermore, gate interactions must be externally switched¹ on and off because the gates affect each other's operation.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited size units, based on several tens of atomic two-level systems, operating in a coherent fashion over sufficiently large time interval to function as parts of a larger classical (dissipative) computer which will not maintain quantum coherent operation over its macroscopic dimensions. We would like these to function as single analog units rather than being composed of many gates.

While in principle in a reversible computational unit input and output spins (qubits) need not be different, for larger units interacting with the external world it may be practically useful to consider input and output separate (or at least not identical). Indeed, the interactions that feed in the input need not necessarily be identical to those interactions/measurements that read off the output.

In light of these considerations we consider in this work a *spatially extended* NOT gate based on two spins: one input and one output. Actually, we have to address a complicated set of problems: can multispin computational units be designed with short-range, two-particle interactions? Can they accomplish logical functions with interactions of the form familiar in condensed matter or other experimental systems? These and similar questions can only be answered by multispin-unit calculations

which will have to be numerical. Analytical results are limited to the simplest gates such as NOT and XOR, the latter studied in Ref. 7, and they provide only a partial picture.

This work is organized as follows. In Section 2 we consider a simple, “textbook” example: the one-qubit NOT gate. It is considered for illustration only and allows us to introduce the notation in a simple setting and exemplify some general ideas. In Section 3 we consider the NOT gate with spatially separated input and output qubits. The interaction Hamiltonian derived for this gate, equation (21) below, establishes that it can be operated by the internal interactions alone so that external-field effects can perhaps be reserved for the clocking of the internal interactions. Furthermore, it suggests the type of local internal interactions to be used in more complicated systems where the computer as a whole is treated as a many-body system with time-independent interactions.

The conventional formulation¹ of quantum computing involves the external on and off switching of the interactions. In Section 4, we show that this requirement can be relaxed and the time dependence be given by other time-dependent interactions (protocols) which are smoother than the on/off shape. Section 4 also offers a summarizing discussion.

2. The simple NOT gate

In this section we consider the NOT gate based on a two-state system. Such a gate has been extensively studied in the literature,¹ so that our discussion is a review intended to set up the notation and illustrate methods useful in more complicated situations. We label by $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the two basis states. The NOT gate corresponds to those interactions which, over the time interval Δt , accomplish the following changes:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow e^{i\alpha} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (1)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow e^{i\beta} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (2)$$

The phases α and β are arbitrary. The unitary matrix U , that corresponds to this evolution, is uniquely determined,

$$U = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\alpha} & 0 \end{pmatrix}. \quad (3)$$

The eigenvalues of U are given by

$$u_1 = e^{i(\alpha+\beta)/2} \quad \text{and} \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad (4)$$

while the eigenvectors, when normalized and regarded as matrix columns, yield the following transformation matrix T which can be used to diagonalize U :

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} \\ e^{i\alpha/2} & -e^{i\alpha/2} \end{pmatrix}. \quad (5)$$

Thus, we have

$$T^\dagger U T = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}. \quad (6)$$

Here the dagger superscript denotes Hermitian conjugation.

We next use the general relation

$$U = e^{-iH\Delta t/\hbar} \quad (7)$$

to identify the time-independent Hamiltonian in the diagonal representation. Relations (4) yield the energy levels:

$$E_1 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}N_1, \quad E_2 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2 + \frac{1}{2}\right), \quad (8)$$

where N_1 and N_2 are arbitrary integers. The Hamiltonian is then obtained from the relation

$$H = T \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} T^\dagger \quad (9)$$

as a certain 2×2 matrix. The latter is conveniently represented in terms of the unit matrix \mathcal{I} and the conventional Pauli matrices $\sigma_x, \sigma_y, \sigma_z$. We get

$$\begin{aligned} H &= \left[-\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{\pi\hbar}{\Delta t}\left(N_1 + N_2 + \frac{1}{2}\right) \right] \mathcal{I} \\ &+ \frac{\pi\hbar}{\Delta t}\left(N_1 - N_2 - \frac{1}{2}\right) \left[\left(\cos \frac{\alpha - \beta}{2}\right) \sigma_x + \left(\sin \frac{\alpha - \beta}{2}\right) \sigma_y \right]. \end{aligned} \quad (10)$$

To effect the gate operation, the interaction must be switched on for the time interval Δt . The constant part of the interaction energy (the part proportional to the unit matrix \mathcal{I}) is essentially arbitrary; it only affects the average phase $\frac{\alpha + \beta}{2}$ of the transformation (1)-(2). Thus this term can be omitted.

The nontrivial part of (10) depends on the integer $N = N_1 - N_2$ which is arbitrary, and on one arbitrary angular variable

$$\gamma = \frac{\alpha - \beta}{2}. \quad (11)$$

Thus we can use the Hamiltonian in the form

$$H = \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2} \right) [(\cos \gamma) \sigma_x + (\sin \gamma) \sigma_y]. \quad (12)$$

For a spin- $\frac{1}{2}$ two-state system such an interaction can be obtained by applying a magnetic field oriented in the XY -plane at an angle γ with the X -axis. The strength of the field is inversely proportional to the desired time interval Δt , and various allowed field values are determined by the choice of N .

We note that during application of the external field the *up* and *down* quantum states in (1)-(2) are *not* the eigenstates of the Hamiltonian. If the time interval Δt

is not short enough, the energy-level splitting $|E_1 - E_2| \propto |N - \frac{1}{2}|$ can result in spontaneous emission which is just one of the undesirable effects destroying quantum coherence. Generally, when implemented in a condensed matter matrix for instance, the two states of the qubit may lie within a spectrum of various other energy levels. In that case, in order to minimize the number of spontaneous transition modes, the best choice of the interaction strength would correspond to minimizing $|E_1 - E_2|$, i.e., to $|N - \frac{1}{2}| = \frac{1}{2}$.

3. The spatially extended NOT gate

In this section we consider a spatially extended NOT gate consisting of two spins: input and output. We will describe these spins by four-state vectors and matrices labeled according to the following self-explanatory convention:

$$\begin{aligned} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} &= a_1 |\uparrow\uparrow\rangle + a_2 |\uparrow\downarrow\rangle + a_3 |\downarrow\uparrow\rangle + a_4 |\downarrow\downarrow\rangle \\ &= a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O \\ &\quad + a_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_4 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O. \end{aligned} \quad (13)$$

Here I and O denote *Input* and *Output*. In what follows we will omit the direct-product symbols \otimes when multiplying expressions with subscripts I and O .

The desired transformation should take any state with $a_3 = a_4 = 0$ into a state with components 1 and 3 equal zero, i.e., *Input up* yields *Output down*. Similarly, any state with $a_1 = a_2 = 0$ should evolve into a state with components 2 and 4 equal zero, corresponding to *Input down* giving *Output up*. The general evolution operator must therefore be of the form

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} \\ U_{21} & U_{22} & 0 & 0 \\ 0 & 0 & U_{33} & U_{34} \\ U_{41} & U_{42} & 0 & 0 \end{pmatrix}, \quad (14)$$

which depends on 16 real parameters. However, one can show that the requirement of unitarity, $U^\dagger U = 1$, imposes 8 conditions so that the number of real parameters is reduced to 8. A lengthy but straightforward algebraic calculation then shows that the following parametrization covers all such unitary matrices:

$$U = \begin{pmatrix} 0 & 0 & e^{i\chi} \sin \Omega & e^{i\beta} \cos \Omega \\ -e^{i(\alpha+\rho-\eta)} \sin \Upsilon & e^{i\rho} \cos \Upsilon & 0 & 0 \\ 0 & 0 & e^{i\delta} \cos \Omega & -e^{i(\beta+\delta-\chi)} \sin \Omega \\ e^{i\alpha} \cos \Upsilon & e^{i\eta} \sin \Upsilon & 0 & 0 \end{pmatrix}. \quad (15)$$

Here all the angular variables are unrestricted although we could limit Ω and Υ to the range $[0, \frac{\pi}{2}]$ without loss of generality.

In order to make the calculation analytically tractable, we will restrict the number of free parameters to four by considering the case

$$U = \begin{pmatrix} 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \end{pmatrix}. \quad (16)$$

This form has been favored for the following reasons. Firstly, the structure of a single phase-factor in each column is similar to that of the two-dimensional matrix encountered in Section 2. Secondly, the form (16) contains Hermitian- U cases ($\beta = -\alpha$, $\rho = 0$ or π , $\delta = 0$ or π). Therefore, the eigenvalues, which are generally on the unit circle for any unitary matrix, may be positioned more symmetrically with respect to the real axis, as functions of the parameters. These observations suggest that an analytical calculation may be possible.

Indeed, the eigenvalues of U turn out to be quite simple:

$$u_1 = e^{i(\alpha+\beta)/2}, \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad u_3 = e^{i\rho}, \quad u_4 = e^{i\delta}. \quad (17)$$

The diagonalizing matrix T made up of the normalized eigenvectors as columns is

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ e^{i\alpha/2} & -e^{i\alpha/2} & 0 & 0 \end{pmatrix}. \quad (18)$$

The next step in the calculation is to identify the energy levels. We chose the notation such that the energies $E_{1,2}$ are identical to (8). The other two energies are given by

$$E_3 = -\frac{\hbar}{\Delta t}\rho + \frac{2\pi\hbar}{\Delta t}N_3, \quad E_4 = -\frac{\hbar}{\Delta t}\delta + \frac{2\pi\hbar}{\Delta t}N_4, \quad (19)$$

The Hamiltonian is then obtained as in Section 2. It is convenient to avoid cumbersome expressions by expressing it in terms of the energies; the latter will be replaced by explicit expressions (8), (19) when needed. The resulting 4×4 matrix has been expressed in terms of the direct products involving the unit matrices and the Pauli matrices of the *Input* and *Output* two-state systems. This calculation is straightforward but rather lengthy. We only report the result:

$$\begin{aligned} H &= \frac{1}{4}(2E_1 + 2E_2 + E_3 + E_4) + \frac{1}{4}(E_3 - E_4)(\sigma_{zI} - \sigma_{zO}) \\ &+ \frac{1}{4}(2E_1 + 2E_2 - E_3 - E_4)\sigma_{zI}\sigma_{zO} \\ &+ \frac{1}{4}(E_1 - E_2)\left(\cos\frac{\alpha - \beta}{2}\right)(\sigma_{xI}\sigma_{xO} - \sigma_{yI}\sigma_{yO}) \\ &+ \frac{1}{4}(E_1 - E_2)\left(\sin\frac{\alpha - \beta}{2}\right)(\sigma_{xI}\sigma_{yO} + \sigma_{yI}\sigma_{xO}). \end{aligned} \quad (20)$$

As in Section 2, we note that the constant part of the Hamiltonian can be changed independently of the other coupling constants and it can be discarded. Recall that we can generally vary the integers $N_{1,2,3,4}$ and the variables $\alpha, \beta, \rho, \delta$. The “constant” part is in fact proportional to $\mathcal{I}_I \otimes \mathcal{I}_O$. However, we avoid this cumbersome notation and present the terms in the Hamiltonian in a more physically transparent form.

The Hamiltonian in (20) has also terms linear in the Pauli matrices (in the spin components for spin systems). These correspond to interactions with externally applied fields which in fact must be of opposite direction for the *Input* and *Output* spins. We try to avoid such interactions: hopefully, external fields will only be used for “clocking” of the computation, i.e., for controlling the internal interactions of the *Input* and *Output* two-state systems. Thus, we will assume that $E_3 = E_4$ so that there are no terms linear in the spin components, in the Hamiltonian.

Among the remaining interaction terms, the term involving the z -components in the product form $\sigma_{zI}\sigma_{zO}$ ($\equiv \sigma_{zI} \otimes \sigma_{zO}$), has an arbitrary coefficient, say, $-\mathcal{E}$. The terms of order two in the x and y components have free parameters similar to those in (11)-(12) in Section 2. The final expression is

$$\begin{aligned} H = & -\mathcal{E}\sigma_{zI}\sigma_{zO} \\ & + \frac{\pi\hbar}{2\Delta t} \left(N - \frac{1}{2} \right) \left[(\cos \gamma) (\sigma_{xI}\sigma_{xO} - \sigma_{yI}\sigma_{yO}) \right. \\ & \left. + (\sin \gamma) (\sigma_{xI}\sigma_{yO} + \sigma_{yI}\sigma_{xO}) \right]. \end{aligned} \quad (21)$$

Here $N = N_1 - N_2$ must be integer. In order to minimize the spread of the energies E_1 and E_2 we could choose $|N - \frac{1}{2}| = \frac{1}{2}$ as in Section 2. Recall that we already have $E_3 = E_4$. Actually, the energy levels of the Hamiltonian in the notation (21) are

$$E_1 = -\mathcal{E} + \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2} \right), \quad E_2 = -\mathcal{E} - \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2} \right), \quad E_{3,4} = \mathcal{E}. \quad (22)$$

Thus further degeneracy (of three levels but not all four) can be achieved by varying the parameters.

4. Time-dependent interactions. Discussion

The form of the interactions in (21) is quite unusual as compared to the traditional spin-spin interactions in condensed matter models. The latter usually are based on the uniaxial (Ising) interaction proportional to $\sigma_z\sigma_z$, or the planar XY -model interaction proportional to $\sigma_x\sigma_x + \sigma_y\sigma_y$, or the isotropic (scalar-product) Heisenberg interaction. The spin components here are those of two different spins (not marked). The interaction (21) involves an unusually high degree of anisotropy in the system. The x and y components are coupled in a tensor form which presumably will have to be realized in a medium with well-defined directionality, possibly, a crystal.

All the interaction Hamiltonians considered thus far were constant for the duration of the gate operation. They must be externally controlled. However, we note that the application of the interaction need not be limited to the time-dependence which is an abrupt on/off switching. Indeed, we can modify the time dependence according to

$$H(t) = f(t)H, \quad (23)$$

where we use the same symbol H for both the original time-independent interaction Hamiltonian such as (21) and the new, time-dependent one, $H(t)$. The latter involves the “protocol” function $f(t)$. The shape of this function, nonzero during the operation of the gate from time t to time $t + \Delta t$, can be smooth.

For Hamiltonians involving externally applied fields, such as (12), it may be important to have a constant plus an oscillatory components (corresponding to constant and electromagnetic-wave magnetic fields, for instance). However, the protocol function must satisfy

$$\int_t^{t+\Delta t} f(t') dt' = \Delta t, \quad (24)$$

and therefore it cannot be purely oscillatory; it must have a constant or other contribution to integrate to a nonzero value in accordance with (24).

The possibility of the modification (23) follows from the fact that the general relation

$$U = \left[e^{-i \int_t^{t+\Delta t} H(t') dt' / \hbar} \right]_{\text{time-ordered}} \quad (25)$$

does not actually require time ordering as long as the Hamiltonian commutes with itself at different times. This condition is satisfied by (23). Furthermore, if the Hamiltonian can be written as a sum of commuting terms then each term can be multiplied by its own protocol function. Interestingly, the Hamiltonian of the “paramagnetic resonance” NOT gate, reviewed by DiVincenzo in Refs. 1, is not of this form. It contains a constant part and an oscillatory part but they do not commute. Note that the term proportional to \mathcal{E} in (21) commutes with the rest of that Hamiltonian. The terms proportional to $\cos \gamma$ and $\sin \gamma$ do not commute with each other though. Rather, they anticommute, in (21), as such terms do in (12).

In summary, we have derived expressions for the interaction Hamiltonians appropriate for the NOT gate operation in two-state systems. The expressions obtained will be useful in identifying materials where there is hope of actually realizing such gates, in writing down model Hamiltonians for more complicated, multispin configurations, and in studying these gates as individual components, for instance, with dissipation added.

Acknowledgements

The work at Clarkson University has been supported in part by US Air Force grants, contract numbers F30602-96-1-0276 and F30602-97-2-0089. The work at Rome

Laboratory has been supported by the AFOSR Exploratory Research Program and by the Photonics in-house Research Program. This financial assistance is gratefully acknowledged.

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